Master in Photonics – "PHOTONICS BCN"
Master ERASMUS Mundus "EuroPhotonics"

MASTER THESIS PROPOSAL

Dates: April 2021 - September 2022

Laboratory: Attoscience and Ultrafast Optics
Institution: ICFO – The Institute of Photonics Sciences
City, Country: Barcelona, Spain

Title of the master thesis: Molecular structural imaging with single-electron diffraction

Name of the master thesis supervisor and co-supervisor:
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Keywords: attosecond science, electron diffraction, structural identification, molecular dynamics, diffraction imaging

Summary of the subject (maximum 1 page):
How does a molecule dissociate, and how does its chemical reaction occur? While the geometric structures of many biologically-important molecules are well studied by conventional electron and X-ray diffraction, the reaction dynamics of many biologically-important molecules are still unknown. One such example is trans-cis photoisomerization of photo-switchable molecules which e. g. help regulate vision and metabolism.
At a most fundamental level, the quantum nature of electronic correlations and coupled interactions of electrons and nuclei drive the chemical reactions of a molecule. Thus, our aim is to get an insight of the electronic and nuclear motion on their native time scales and to possibly control their dynamics. However, tracking such ultrafast dynamics requires imaging techniques which can provide a clean snapshot of molecular structure with atomic spatial (i.e. Ångstrom; 1 Å = 10-10 m) and temporal (i.e. femtosecond; 1 fs = 10-15 s) resolution. In our group, such resolution is achieved by laser-induced electron diffraction (LIED). Thereby an intense, femtosecond laser pulse is utilized to liberate an electron from a molecule through quantum tunnel ionization. The emitted electron is then accelerated and returned by the oscillating electric field of the laser pulse to subsequently

elastically scatter and diffract against the molecular ion. The scattered electrons are detected in coincidence with the ion of interest by a high-resolution particle detector. With sub-atomic picometre and attosecond resolution, the molecular structure can directly be retrieved from the three-dimensional momentum distribution of the scattered electrons.

LIED imaging has successfully uncovered deprotonation reactions in molecules, the strong nuclear-electronic coupling via the Renner-Teller effect, and the structural identification of many small gas-phase molecules. An exciting opportunity now exists to extend LIED imaging to more complex, larger polyatomic molecules which possess a rich variety of chemistry. You will be dealing with the theory and method of LIED to directly identify and distinguish the static structures of trans- and cis- isomers. This will provide the starting and end points of the trans-cis photoisomerization reaction, the data from which will then be utilized to identify the transient structures in future time-resolved pump-probe measurements of isomerization.

Additional information:

***Required skills:** Physics or Physical Chemistry undergraduate, problem-solving, critical-thinking, quick learner, ability to work independently and in a team, basic computer programming.

***Miscellaneous:**